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Supporting Information for Szyperski *et al.* (2002) *Proc. Natl. Acad. Sci. USA* 99 (12), 8009–8014. (10.1073/pnas.122224599).

Supporting Figure 13

Fig. 13. Sequential resonance assignment based on 3D $\underline{H}^{a/b}\underline{C}^{a/b}(\text{CO})\text{NHN}$ / 3D $\underline{H}^{a/b}\underline{C}^{a/b}\text{COHA}$ combined with 3D $\text{HNN}<\underline{CA},\underline{CO}>$ (see Fig. 2). The amino acid residue on which the NMR signal was detected is indicated at the bottom of the strips. (A) Matching of $w_1(^{13}\text{C}^{a/b}/^1\text{H}^{a/b})$ peak patterns in 3D $\underline{H}^{a/b}\underline{C}^{a/b}\text{COHA}$ (strips labeled with "a") and 3D $\underline{H}^{a/b}\underline{C}^{a/b}(\text{CO})\text{NHN}$ ("b") yields putative intraresidue $^1\text{H}^{a/b}/^{13}\text{C}^{a/b}$ - $^{13}\text{C}=\text{O}$ correlations: on the strips taken from 3D $\underline{H}^{a/b}\underline{C}^{a/b}\text{COHA}$ the $^{13}\text{C}=\text{O}$ chemical shift is indicated. (B) 3D $\text{HNN}<\underline{CA},\underline{CO}>$ yields the sequential $^{13}\text{C}=\text{O}$ - $^{13}\text{C}^a$ correlations: the carbonyl chemical shifts have to match those shown in A, and are indicated on the left of the figure. Proton and carbon chemical shifts are given in ppm and relative to 2,2-dimethyl-2-silapentane-5-sulfonate (DSS).

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